Quantum Mechanics 3 - Class Exercise 1

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Administration

- **Name:** Jordan (Yarden) Flitter.
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- **Office hour:** shall be taken place on Zoom. Please fill in your preferences in the *Doodle poll*. Please send me an email that you wish to attend an office hour (at least 24 hours before it is scheduled), or otherwise the office hour for that week will be canceled.
- **Recitations:** My notes shall be uploaded to Moodle before each recitation.
- **Course grade:** (see course policy at the website)
  - 10% homework assignments. Students are required to grade themselves by a weekly deadline after the official solution has been uploaded to the course website. One homework, with the lowest grade, will not be taken into account in computing the average. Please note:
    - Submission of HW assignment without grading it will be considered as if the HW assignment has not been submitted, and no credit will be given for that HW assignment.
    - The HW deadlines are strict! Requests for postponing the deadline will be declined, except for particular circumstances (Miluim, special family occasions, etc...) and only if the request has been sent to the staff members before the deadline.
  - 90% final assignment (50% for work and 40% for oral exam).

Question 1

Consider a two-state system described by the Hamiltonian $\hat{H} = \frac{E}{2}\hat{\sigma}_z + \epsilon\cos(\omega t)\,\hat{\sigma}_x$. If the initial state is $|1\rangle = \begin{bmatrix}1\\0\end{bmatrix}$ at $t = 0$, what is the transition probability to $|2\rangle = \begin{bmatrix}0\\1\end{bmatrix}$ as a function of time? Assume that $|\epsilon| \ll |E|$, $|E - \hbar\omega| \ll |E + \hbar\omega|$.

Solution

Recall the famous Pauli matrices

$$\hat{\sigma}_x = \begin{bmatrix}0 & 1\\1 & 0\end{bmatrix} \qquad \hat{\sigma}_y = \begin{bmatrix}0 & -i\\i & 0\end{bmatrix} \qquad \hat{\sigma}_z = \begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}. \tag{1}$$

The state of the system can be expressed as $|\psi(t)\rangle = a(t)|1\rangle + b(t)|2\rangle$ and its evolution is governed by the Schrödinger equation,

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle, \tag{2}$$

which in our case is

$$i\hbar\begin{bmatrix}\dot{a}\\\dot{b}\end{bmatrix} = \begin{bmatrix}E/2 & \epsilon\cos(\omega t)\\\epsilon\cos(\omega t) & -E/2\end{bmatrix}\begin{bmatrix}a\\b\end{bmatrix}, \tag{3}$$

or

$$\dot{a} = -i\frac{E}{2\hbar}a - i\frac{\epsilon}{\hbar}\cos(\omega t)\,b \tag{4}$$

$$\dot{b} = i\frac{E}{2\hbar}b - i\frac{\epsilon}{\hbar}\cos(\omega t)\,a. \tag{5}$$

These coupled differential equations can be simplified if we work in the interaction picture, where Schrödinger equation becomes

$$i\hbar\frac{\partial}{\partial t}|\psi_I\rangle = \hat{V}_I|\psi_I\rangle. \tag{6}$$

This picture is more convenient for solving the differential equations because the on-diagonal elements of $\hat{V}_I$ are guaranteed to be zero. Let's convince ourself that this is indeed the case. In class you saw the definition for $\hat{V}_I$:

$$\hat{V}_I(t) \equiv \hat{U}_0^\dagger(t,t_0)\left(\hat{H}(t) - \hat{H}_0\right)\hat{U}_0(t,t_0), \tag{7}$$

where

$$\hat{H}_0 = \begin{bmatrix}E/2 & 0\\0 & -E/2\end{bmatrix}, \qquad \hat{U}_0(t,t_0) = \mathrm{e}^{-i\hat{H}_0(t-t_0)/\hbar} = \begin{bmatrix}\mathrm{e}^{-iE(t-t_0)/2\hbar} & 0\\0 & \mathrm{e}^{+iE(t-t_0)/2\hbar}\end{bmatrix}. \tag{8}$$

Thus (here I set $t_0 = 0$),

$$\begin{aligned}\hat{V}_I &= \begin{bmatrix}\mathrm{e}^{+iEt/2\hbar} & 0\\0 & \mathrm{e}^{-iEt/2\hbar}\end{bmatrix}\begin{bmatrix}0 & \epsilon\cos(\omega t)\\\epsilon\cos(\omega t) & 0\end{bmatrix}\begin{bmatrix}\mathrm{e}^{-iEt/2\hbar} & 0\\0 & \mathrm{e}^{+iEt/2\hbar}\end{bmatrix}\\ &= \begin{bmatrix}0 & \epsilon\mathrm{e}^{+iEt/\hbar}\cos(\omega t)\\\epsilon\mathrm{e}^{-iEt/\hbar}\cos(\omega t) & 0\end{bmatrix} = \begin{bmatrix}0 & V\\V^* & 0\end{bmatrix},\end{aligned} \tag{9}$$

where I defined $V \equiv \epsilon\mathrm{e}^{+iEt/\hbar}\cos(\omega t)$.

Thus, Eq. (6) in matrix form is

$$i\hbar\begin{bmatrix}\dot{a}_I\\ \dot{b}_I\end{bmatrix}=\begin{bmatrix}0 & V\\ V^* & 0\end{bmatrix}\begin{bmatrix}a_I\\ b_I\end{bmatrix}, \tag{10}$$

or

$$\dot{a}_I=-i\frac{V}{\hbar}b_I, \tag{11}$$

$$\dot{b}_I=-i\frac{V^*}{\hbar}a_I. \tag{12}$$

Taking the derivative of Eq. (12) and plugging Eq. (11) yields

$$\ddot{b}_I-\frac{\dot{V}^*}{V^*}\dot{b}_I+\frac{|V|^2}{\hbar^2}b_I=0. \tag{13}$$

Let us look closely on the definition of V:

$$V\equiv\epsilon\mathrm{e}^{+iEt/\hbar}\cos(\omega t)=\frac{\epsilon}{2}\left(\mathrm{e}^{+i(E/\hbar+\omega)t}+\mathrm{e}^{+i(E/\hbar-\omega)t}\right)\approx\frac{\epsilon}{2}\mathrm{e}^{+i(E/\hbar-\omega)t}=\frac{\epsilon}{2}\mathrm{e}^{+i\delta t}, \tag{14}$$

where in the last step I defined $\delta\equiv E/\hbar-\omega$. The approximation I made in Eq. (14) might look odd. This is known as the "rotating wave approximation". This approximation is justified by imagining that the higher frequency terms oscillate very rapidly and thus give zero average contribution on the timescales of interest. In your HW, you will show that this approximation is indeed justified as long as $|\epsilon|\ll|E|$ and $|\delta|\ll|E/\hbar+\omega|$. Thus, with the rotating wave approximation Eq. (13) becomes

$$\ddot{b}_I+i\delta\dot{b}_I+\frac{\epsilon^2}{4\hbar^2}b_I=0. \tag{15}$$

We guess $b_I(t)\sim\mathrm{e}^{\alpha t}$ and plug this guess in Eq. (15). This leads to the quadratic equation

$$\alpha^2+i\delta\alpha+\frac{\epsilon^2}{4\hbar^2}=0, \tag{16}$$

which has the solution

$$\alpha=\frac{-i\delta\pm i\Omega}{2},\qquad \Omega\equiv\sqrt{\delta^2+\frac{\epsilon^2}{\hbar^2}}. \tag{17}$$

Thus, the solution for $b_I(t)$ is

$$b_I(t)=\mathrm{e}^{-i\delta t/2}\left(A\mathrm{e}^{i\Omega t/2}+B\mathrm{e}^{-i\Omega t/2}\right), \tag{18}$$

where A and B are constants. In order to find A and B, we would need to move back to Schrödinger picture. The relation between Schrödinger picture and the interaction picture is given by

$$|\psi_I(t)\rangle\equiv U_0^\dagger(t,0)|\psi(t)\rangle\implies|\psi(t)\rangle=U_0(t,0)|\psi_I(t)\rangle, \tag{19}$$

or

$$a(t)=\mathrm{e}^{-iEt/2\hbar}a_I(t), \tag{20}$$

$$b(t)=\mathrm{e}^{iEt/2\hbar}b_I(t). \tag{21}$$

Combining Eqs. (18) and (21), we find

$$b(t)=\mathrm{e}^{i\omega t/2}\left(A\mathrm{e}^{i\Omega t/2}+B\mathrm{e}^{-i\Omega t/2}\right). \tag{22}$$

Since the system starts at $|1\rangle$ at $t=0$, $b\left(t=0\right)=0$, and therefore $A=-B$. The derivative of $b_I\left(t\right)$ is

$$\dot{b}_I\left(t\right)=iA\mathrm{e}^{-i\delta t/2}\left[-i\delta\sin\left(\frac{\Omega t}{2}\right)+\Omega\cos\left(\frac{\Omega t}{2}\right)\right]. \tag{23}$$

According to Eq. (12) this means that

$$a_I\left(t\right)=-\frac{2A\hbar}{\epsilon}\mathrm{e}^{i\delta t/2}\left[-i\delta\sin\left(\frac{\Omega t}{2}\right)+\Omega\cos\left(\frac{\Omega t}{2}\right)\right]. \tag{24}$$

and therefore

$$a\left(t\right)=-\frac{2A\hbar}{\epsilon}\mathrm{e}^{-i\omega t/2}\left[-i\delta\sin\left(\frac{\Omega t}{2}\right)+\Omega\cos\left(\frac{\Omega t}{2}\right)\right], \tag{25}$$

But the initial conditions set $|a\left(t=0\right)|=1$ and thus

$$A=\frac{\epsilon}{2\hbar\Omega}. \tag{26}$$

Therefore

$$b\left(t\right)=i\frac{\epsilon}{\hbar\Omega}\mathrm{e}^{i\omega t/2}\sin\left(\frac{\Omega t}{2}\right), \tag{27}$$

and the probability to find the system at $|2\rangle$ at time t is

$$\boxed{P_2\left(t\right)=|b\left(t\right)|^2=\left(\frac{\epsilon}{\hbar\Omega}\right)^2\sin^2\left(\frac{\Omega t}{2}\right)}. \tag{28}$$

So the system oscillates between its states. The frequency of the oscillations, Ω, is called the Rabi frequency.

Note: Notice that $|a\left(t\right)|^2+|b\left(t\right)|^2\neq 1$. Why do you think we ended up with this result?

Question 2

Consider a free particle with mass m that was prepared as a Gaussian

$$\psi\left(x,t=0\right)=A\mathrm{e}^{-x^{2}/4\sigma^{2}}. \tag{29}$$

What is the uncertainty in the position at time $t>0$?

Solution

The uncertainty is

$$\Delta x\left(t\right)=\sqrt{\langle x^{2}\left(t\right)\rangle-\langle x\left(t\right)\rangle^{2}}. \tag{30}$$

At $t=0$ the particle's probability distribution is a Gaussian with a standard deviation σ,

$$P\left(x,t=0\right)=\left|\psi\left(x,t=0\right)\right|^{2}=\left|A\right|^{2}\mathrm{e}^{-x^{2}/2\sigma^{2}}, \tag{31}$$

and this is also the uncertainty in the particle's position at $t=0$, $\Delta x\left(t=0\right)=\sigma$.

Note: Do not confuse the standard deviation of the wave-function with the standard deviation of the probability distribution. Only the latter is physical!

Our motivation is to find $P\left(x,t\right)=\left|\psi\left(x,t\right)\right|^{2}$ and then to calculate the uncertainty at time $t>0$. The particle is free, hence its state experiences evolution in time that is generated by the Hamiltonian $\hat{H}=\hat{p}^{2}/2m$. Therefore the wave-function in time t is given by

$$\psi\left(x,t\right)=\langle x|\psi\left(t\right)\rangle=\langle x|\mathrm{e}^{-i\frac{\hat{p}^{2}t}{2m\hbar}}|\psi\left(t=0\right)\rangle. \tag{32}$$

Since the evolution operator is diagonal only in momentum-basis, we may use the completeness relation

$$\hat{1}=\int_{-\infty}^{\infty}|p\rangle\langle p|dp, \tag{33}$$

and plug it in the expression for $\psi\left(x,t\right)$:

$$\begin{aligned}\psi\left(x,t\right) &= \langle x|\mathrm{e}^{-i\frac{\hat{p}^{2}t}{2m\hbar}}\hat{1}|\psi\left(t=0\right)\rangle=\langle x|\mathrm{e}^{-i\frac{\hat{p}^{2}t}{2m\hbar}}\int_{-\infty}^{\infty}|p\rangle\langle p|dp|\psi\left(t=0\right)\rangle\\ &= \langle x|\int_{-\infty}^{\infty}\mathrm{e}^{-i\frac{p^{2}t}{2m\hbar}}|p\rangle\langle p|dp|\psi\left(t=0\right)\rangle=\int_{-\infty}^{\infty}\langle x|p\rangle\langle p|\psi\left(t=0\right)\rangle\mathrm{e}^{-i\frac{p^{2}t}{2m\hbar}}dp.\end{aligned} \tag{34}$$

Let us use another completeness relation,

$$\hat{1}=\int_{-\infty}^{\infty}|x'\rangle\langle x'|dx', \tag{35}$$

and plug it in our expression

$$\begin{aligned}\psi\left(x,t\right) &= \int_{-\infty}^{\infty}\langle x|p\rangle\langle p|\hat{1}|\psi\left(t=0\right)\rangle\mathrm{e}^{-i\frac{p^{2}t}{2m\hbar}}dp=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\langle x|p\rangle\langle p|x'\rangle\langle x'|\psi\left(t=0\right)\rangle\mathrm{e}^{-i\frac{p^{2}t}{2m\hbar}}dpdx'\\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\langle x|p\rangle\langle p|x'\rangle\psi\left(x',t=0\right)\mathrm{e}^{-i\frac{p^{2}t}{2m\hbar}}dpdx'.\end{aligned} \tag{36}$$

We will use also use the relations

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\mathrm{e}^{ipx/\hbar}, \qquad \langle p|x\rangle = \langle x|p\rangle^* = \frac{1}{\sqrt{2\pi\hbar}}\mathrm{e}^{-ipx/\hbar}. \tag{37}$$

Thus

$$\begin{aligned}\psi\left(x,t\right) &= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\psi\left(x',t=0\right)\mathrm{e}^{-\frac{i}{\hbar}\left[\frac{p^2t}{2m}-p(x-x')\right]}dpdx' \\ &= \frac{A}{2\pi\hbar}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\mathrm{e}^{-\frac{i}{\hbar}\left[\frac{p^2t}{2m}-p(x-x')\right]-\frac{x'^2}{4\sigma^2}}dpdx'.\end{aligned} \tag{38}$$

We perform first the x' integral using the identity

$$\int_{-\infty}^{\infty}\mathrm{e}^{-ax^2+bx}dx = \sqrt{\frac{\pi}{a}}\mathrm{e}^{b^2/4a}. \tag{39}$$

$$\psi\left(x,t\right) = \frac{A\sigma}{\sqrt{\pi}\hbar}\int_{-\infty}^{\infty}\mathrm{e}^{\frac{i}{\hbar}px}\mathrm{e}^{-\left(\frac{it}{2m\hbar}+\frac{\sigma^2}{\hbar^2}\right)p^2}dp. \tag{40}$$

Let us pause for a moment and notice that Eq. (40) is the expression for inverse Fourier transform of $\tilde{\psi}\left(p,t\right)$ which is given by

$$\tilde{\psi}\left(p,t\right) \propto \mathrm{e}^{-\left(\frac{it}{2m\hbar}+\frac{\sigma^2}{\hbar^2}\right)p^2}. \tag{41}$$

Therefore, the probability that the particle will posses a momentum p at time t is

$$P\left(p,t\right) = \left|\tilde{\psi}\left(p,t\right)\right|^2 \propto \mathrm{e}^{-2\frac{\sigma^2p^2}{\hbar^2}}. \tag{42}$$

This probability is also in the form of a Gaussian but with uncertainty of

$$\boxed{\Delta p\left(t\right) = \frac{\hbar}{2\sigma}}. \tag{43}$$

Notice that this uncertainty is independent of time!

We now continue with the p integral in Eq. (40). Using Eq. (39) we find

$$\psi\left(x,t\right) = \frac{A}{\sqrt{1+\frac{i\hbar t}{2m\sigma^2}}}\exp\left(-\frac{x^2}{4\sigma^2+\frac{2i\hbar t}{m}}\right), \tag{44}$$

and the probability distribution is

$$P\left(x,t\right) = \left|\psi\left(x,t\right)\right|^2 = \frac{|A|^2}{\sqrt{1+\left(\frac{\hbar t}{2m\sigma^2}\right)^2}}\exp\left(-\frac{x^2}{2\sigma^2\left[1+\left(\frac{\hbar t}{2m\sigma^2}\right)^2\right]}\right). \tag{45}$$

We learn from Eq. (45) that the probability distribution remains Gaussian for $t>0$ but with a standard deviation of

$$\boxed{\Delta x\left(t\right) = \sigma\sqrt{1+\left(\frac{\hbar t}{2m\sigma^2}\right)^2}}. \tag{46}$$

The standard deviation is a monotonous increasing function of time. The Gaussian remains centered at $x = 0$ but it spreads with time and the uncertainty in the particle's position becomes greater!

Let us make a sanity check by calculating the product of the uncertainties in position and momentum:

$$\Delta x\left(t\right)\Delta p\left(t\right) = \sigma\sqrt{1+\left(\frac{\hbar t}{2m\sigma^2}\right)^2}\cdot\frac{\hbar}{2\sigma} = \frac{\hbar}{2}\sqrt{1+\left(\frac{\hbar t}{2m\sigma^2}\right)^2} \geq \frac{\hbar}{2}, \tag{47}$$

where equality holds only at $t = 0$.

Question 3

Build explicitly a quantum state which would describe, as closely as possible, a classical particle moving with a constant velocity (in 3D).

Solution

Firstly, we know that each quantum particle must obey the uncertainty principle $\Delta x_i \Delta p_j \geq \frac{\hbar}{2}\delta_{ij}$. Therefore, the "most classical" particle is characterized by minimal uncertainty

$$\Delta x_i \Delta p_j = \frac{\hbar}{2}\delta_{ij}. \tag{48}$$

What kind of a wave-function obeys such relation? Our old friend the Gaussian! We can see from Eq. (47) that a wave-function such as Eq. (29) indeed satisfies Eq. (48). Thus, for a 3D particle we guess[1]

$$\psi\left(\vec{r}\right) = A\mathrm{e}^{-\frac{x^2}{4\sigma^2}-\frac{y^2}{4\sigma^2}-\frac{z^2}{4\sigma^2}}. \tag{49}$$

Yet, we saw in the former problem that such a wave-function remains centered at the origin, so Eq. (49) only corresponds to a classical particle in its rest frame. How the classical particle's wave-function looks like in any other reference frame? It is instructive to prove that if we add to the Gaussian a phase $m\vec{v}\cdot\vec{r}/\hbar$ then its center moves with velocity $\vec{v}$.

$$\psi\left(\vec{r}\right) \to \mathrm{e}^{i\frac{m\vec{v}\cdot\vec{r}}{\hbar}}\psi\left(\vec{r}\right) = A\mathrm{e}^{-\frac{r^2}{4\sigma^2}+i\frac{m\vec{v}\cdot\vec{r}}{\hbar}}. \tag{50}$$

Ok, just because you asked for it!

For simplicity, we work in 1D (although it is straightforward to extend our calculations to 3D). From Eq. (38) we see that an additional phase of $mvx/\hbar$ results

$$\begin{aligned}\psi\left(x,t\right) &= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\psi\left(x',t=0\right)\mathrm{e}^{-\frac{i}{\hbar}\left[\frac{p^2t}{2m}-p(x-x')\right]}dpdx' \\ &= \frac{A}{2\pi\hbar}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\mathrm{e}^{-\frac{i}{\hbar}\left[\frac{p^2t}{2m}-p(x-x')\right]-\frac{x'^2}{4\sigma^2}+\frac{i}{\hbar}mvx'}dpdx'.\end{aligned} \tag{51}$$

This changes the coefficient b in Eq. (39),

$$b = -\frac{i}{\hbar}p \to -\frac{i}{\hbar}\left(p-mv\right), \tag{52}$$

and by performing the x' integral in Eq. (51) we get

$$\begin{aligned}\psi\left(x,t\right) &= \frac{A\sigma}{\sqrt{\pi}\hbar}\int_{-\infty}^{\infty}\mathrm{e}^{\frac{i}{\hbar}px}\mathrm{e}^{-\frac{it}{2m\hbar}p^2-\frac{\sigma^2}{\hbar^2}(p-mv)^2}dp \\ &= \int_{-\infty}^{\infty}\mathrm{e}^{\frac{i}{\hbar}px}\mathrm{e}^{\frac{itmv^2}{2\hbar}}\mathrm{e}^{-\frac{ivt}{\hbar}p}\underbrace{\frac{A\sigma}{\sqrt{\pi}\hbar}\mathrm{e}^{-\left(\frac{it}{2m\hbar}+\frac{\sigma^2}{\hbar^2}\right)(p-mv)^2}}_{\tilde{\psi}(p-mv,t)}dp.\end{aligned} \tag{53}$$

[1] Note that for simplicity we have chosen the same initial uncertainty σ for each direction, but a different uncertainty in each direction would also satisfy Eq. (48).

As before, we can now identify the Fourier transformation of the wave-function, $\tilde{\psi}(p,t)$. We see that the velocity v changes $\tilde{\psi}(p,t)$ according to

$$\tilde{\psi}(p,t) \to \mathrm{e}^{\frac{itmv^2}{2\hbar}} \mathrm{e}^{-\frac{ivt}{\hbar}p} \tilde{\psi}(p-mv,t)\,. \tag{54}$$

The first phase is constant and does not depend on p. The second phase is linear with p. Thus, according to Fourier transformations properties, the wave-function changes according to

$$\psi(x,t) \to \mathrm{e}^{\frac{itmv^2}{2\hbar}} \mathrm{e}^{i\frac{mvx}{\hbar}} \psi(x-vt,t)\,, \tag{55}$$

and the probability distribution changes to

$$P(x,t) \to P(x-vt,t)\,. \tag{56}$$

Thus, the Gaussian's center, which remains at $x=0$ when $v=0$, shifts to vt for $t>0$.

What should be the velocity of the particle in order for it to stay classical? We know that as time progresses the uncertainty in the particle's position increases according to $\Delta r(t) = \sigma\sqrt{1+\left(\frac{\hbar t}{2m\sigma^2}\right)^2}$. We would like this uncertainty to be much smaller than the classical distance that the particle has traveled which is vt. Therefore, the particle's velocity has to satisfy

$$v \gg \frac{\sigma}{t}\sqrt{1+\left(\frac{\hbar t}{2m\sigma^2}\right)^2}. \tag{57}$$

For very short times ($t \ll m\sigma^2/\hbar$) the particle has to travel with great velocity in order to be considered as classical, otherwise its position uncertainty will be greater than its classical distance. For late times, the Gaussian has spread considerably and so the particle has to move faster than

$$v \gg \frac{\hbar}{2m\sigma}. \tag{58}$$

Moreover, the particle's uncertainty in momentum also has to be small. This uncertainty is given by Eq. (43) and does not depend on particle's velocity. In order for the particle to be considered as classical, the uncertainty $\Delta p = \hbar/2\sigma$ has to be much smaller than the classical particle's momentum which is mv. This requirement leads to the same condition in Eq. (58).

Note: You should be concerned that our results depend on the particle's speed, which is equivalent to choosing a different reference frame. Yet, we found that the particle has to move very fast in order to be classical. Try to think what happens to the measured time and distance that the particle has traveled, and how this effect can solve this paradox.

Note: I encourage you to go go to Wiki, search for "Wave packet" and go to section "dispersive". You can see there the "semi-classical" particle with your own eyes!